

Matrix continued fraction solution to the relativistic spin-0 Feshbach-Villars equations

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Abstract. The Feshbach-Villars equations, like the Klein-Gordon equation, are relativistic quantum mechanical equations for spin-0 particles. We write the Feshbach-Villars equations into an integral equation form and solve them by applying the Coulomb-Sturmian potential separable expansion method. We consider bound-state problems in a Coulomb plus short range potential. The corresponding Feshbach-Villars Coulomb Green's operator is represented by a matrix continued fraction.

1. Introduction

It is well known that the basic relativistic equation for a spin-0 particle is the Klein-Gordon equation. Probably, it had been formulated first by Schrödinger, but it gave wrong results for the hydrogen atom, so he abandoned it in favor of the non-relativistic formalism. The Klein-Gordon equation was suggested in 1926 by Klein [1] and Gordon [2] as well as by several other people [3, 4, 5]. It can be derived from the relativistic energy-momentum relation using the correspondence principle. It has served as a basic relativistic equation for spin-0 particles in relativistic quantum mechanics and field theory.

The Klein-Gordon equation, however, contradicts some of the postulates of quantum mechanics. In the quantum mechanics it is postulated that the system is completely determined by the wave function and the time evolution of the wave function is determined by the time-dependent Schrödinger equation [6, 7]. The Klein-Gordon equation contains a second derivative in time, therefore to determine the system the wave function is not enough, we need its time derivative as well. So, obviously, the Klein-Gordon equation is not a genuine quantum mechanical equation.

In 1958 Feshbach and Villars rewrote the Klein-Gordon equation into a Hamiltonian form [8]. They split the Klein-Gordon wave function into two components and for the components vector they arrived at a Schrödinger-like equation with first order in time derivative. Although the Feshbach-Villars formalism appear in some advanced quantum mechanics books [9, 10, 11, 12, 13, 14, 15], and they were utilized in gaining deeper insight into relativistic physics of Klein paradox pair production, [16, 17, 18, 19, 20, 21, 22, 23], in exotic atoms [24, 25, 26], used in theoretical considerations [27, 28, 29, 31], study relativistic scattering [32, 32] and optics [33] or demonstrate PT symmetry [34, 35, 36, 37], they were hardly used as a computational tool. The equations look like ordinary coupled differential equations, but the components are coupled by the kinetic energy operator, which makes them very hard to solve.

The aim of this work is to develop a solution method to relativistic quantum mechanical problems by solving the spin-0 Feshbach-Villars (FV0) equations. We adapt a solution method which worked extremely well in the non-relativistic case. First, in Sec. II, we outline the FV0 formalism. Then in Sec. III we recapitulate the solution method for the non-relativistic problems with Coulomb-like potentials. In Sec. IV we present our approach to the FV0 equation. As an example, we choose an attractive Coulomb plus short-range potential problem. This also provides us a convenient test case since the Klein-Gordon hydrogen levels are well known from standard text books. Finally we summarize our findings and draw some conclusions.

2. Feshbach-Villars equations for spin-0 particles

The Klein-Gordon equation with a scalar potential V is given by

$$\left(i\hbar\frac{\partial}{\partial t} - V\right)^2 \Psi = (c^2 p^2 + m^2 c^4) \Psi. \quad (1)$$

In the FV0 formalism the wave function is split into two components

$$\Psi = \phi + \chi, \quad \left(i\hbar\frac{\partial}{\partial t} - V\right) \Psi = mc^2(\phi - \chi), \quad (2)$$

and the components satisfy the coupled equations

$$i\hbar\frac{\partial}{\partial t}\phi = \frac{p^2}{2m}(\phi + \chi) + (mc^2 + V)\phi \quad (3)$$

$$i\hbar\frac{\partial}{\partial t}\chi = -\frac{p^2}{2m}(\phi + \chi) - (mc^2 - V)\chi. \quad (4)$$

By introducing the two-component wave function

$$|\psi\rangle = \begin{pmatrix} \phi \\ \chi \end{pmatrix} \quad (5)$$

and the Hamiltonian

$$H_{FV0} = \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix} \frac{p^2}{2m} + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} mc^2 + \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} V \quad (6)$$

we can write (3) and (4) into a form analogous to the time-dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = H_{FV0}|\psi\rangle, \quad (7)$$

or, for stationary states we may have

$$H_{FV0}|\psi\rangle = E|\psi\rangle. \quad (8)$$

This Hamiltonian looks like a usual coupled-channel Hamiltonian. However, there the channels are coupled by some short-range potential, while here the coupling is due the kinetic energy operator. As we are going to see below, the matrix elements of the kinetic energy operator on a discrete basis representation behaves like n for large n . This is a long-range coupling, it cannot be truncated to a finite basis representation.

3. Solution method for non-relativistic problems

We consider a Coulomb-like potential

$$v_l = v^C + v_l^{(s)}, \quad (9)$$

where l is the angular momentum, $v^C = Ze^2/r$ is the Coulomb potential and $v_l^{(s)}$ is some short-range potential. The bound states are the solutions of the homogeneous Lippmann-Schwinger equation

$$|\psi\rangle = g^C(E)v_l^{(s)}|\psi\rangle, \quad (10)$$

where

$$g^C(E) = (E - p^2/2m - v^C)^{-1} \quad (11)$$

is the the Coulomb Green's operator.

If we approximate the short-range potential by a finite-rank operator, we can solve the equations without any further approximation, provided we can calculate the matrix elements of the Green's operator. In this respect the use of the Coulomb-Sturmian (CS) functions

$$\langle r|n\rangle = \left(\frac{n!}{(n+2l+1)!}\right)^{1/2} e^{-br}(2br)^{l+1}L_n^{2l+1}(2br), \quad (12)$$

where L is the Laguerre polynomial and b is a parameter, is particularly advantageous. The CS functions form a basis. With $\langle r|\tilde{n}\rangle = \langle r|n\rangle/r$ we have:

$$\langle \tilde{n}|n'\rangle = \delta_{nn'} \quad (13)$$

and

$$1 = \lim_{N \rightarrow \infty} \sum_{n=0}^N |n\rangle \langle \tilde{n}| = \lim_{N \rightarrow \infty} \sum_{n=0}^N |\tilde{n}\rangle \langle n|. \quad (14)$$

The simple form of CS basis allow an exact and analytic calculations of the matrix elements:

$$\langle n|n'\rangle = \begin{cases} (n+l+1)/b & \text{if } n = n', \\ -\sqrt{n'(n'+2l+1)}/(2b) & \text{if } n' = n+1, \\ 0 & \text{otherwise,} \end{cases} \quad (15)$$

and

$$\langle n|\frac{p^2}{2m}|n'\rangle = \begin{cases} (n+l+1)b/(2m) & \text{if } n = n', \\ \sqrt{n'(n'+2l+1)}b/(4m) & \text{if } n' = n+1, \\ 0 & \text{otherwise.} \end{cases} \quad (16)$$

Thus the operator $J = E - p^2/2m - v^C$ is an infinite tridiagonal matrix on the CS basis. An important result of Refs. [38, 39] is that for infinite tridiagonal matrices the $N \times N$ part of the inverse, or the Green's matrix, is given by

$$\underline{g}^C = (\underline{J} - \delta_{iN}\delta_{jN}J_{N,N+1}C_{N+1}J_{N+1,N})^{-1}, \quad (17)$$

where \underline{g}^C and \underline{J} are $N \times N$ matrices and C is a continued fraction. So, basically, \underline{g}^C is almost the inverse of \underline{J} , only the right-down corner of \underline{J} is modified by a continued

fraction. The continued fraction is constructed from the higher-index elements of J and is defined by the recursion relation

$$C_{N+1} = (J_{N+1,N+1} - J_{N+1,N+2}C_{N+2}J_{N+2,N+1})^{-1}. \quad (18)$$

Over many years various finite-rank expansion methods for approximating $v^{(s)}$ have been used. In a recent work we proposed a simple, straightforward, yet very efficient approximation scheme [40]. It amounts of representing the short-range potential in a larger basis, invert the potential matrix, truncate to a smaller basis, and then invert it back. This way we achieve a low-rank representation of the potential operator that contains the relevant information from the larger basis. Even a low-rank representation gives very good figures, while higher-rank representations give extremely accurate results.

This method of solving problems of non-relativistic quantum mechanics through integral equations has been extended further for solving more challenging problems like the three-body Faddeev integral equations with Coulomb potentials [41, 42].

4. Relativistic spin-0 particles in Coulomb-like potentials

We consider a relativistic spin-0 particle in a Coulomb-like potential. Its FV0 Hamiltonian is given by

$$H_{FV0} = H_{FV0}^C + v_{FV0}^{(s)} \quad (19)$$

with

$$H_{FV0}^C = \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix} \frac{p^2}{2m} + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} mc^2 + \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} v^C \quad (20)$$

and

$$v_{FV0}^{(s)} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} v_l^{(s)}. \quad (21)$$

Analogous to the non-relativistic case, we can cast the eigenvalue problem of the two-component wave function into a Lippmann-Schwinger form

$$|\psi\rangle = g_{FV0}^C(E) v_{FV0}^{(s)} |\psi\rangle, \quad (22)$$

where

$$g_{FV0}^C(E) = [E - H_{FV0}^C]^{-1}. \quad (23)$$

Since $v_{FV0}^{(s)}$ is just a diagonal 2×2 matrix with $v_l^{(s)}$ in the diagonal, we can approximate $v_l^{(s)}$ as before in the non-relativistic case.

In the CS basis the constant, the Coulomb potential and the kinetic energy operators are either diagonal or tridiagonal infinite matrices. So, for

$$J_{FV0} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} E - \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix} \frac{p^2}{2m} - \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} mc^2 - \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} v^C, \quad (24)$$

the infinite tridiagonal structure is superimposed by some 2×2 matrix structures. In other words, J_{FV0} is infinite block-tridiagonal with 2×2 matrix blocks. The same arguments which resulted in Eq. (17) is applicable here and leads to a similar expression, only $J_{i,j}$'s should be understood as 2×2 matrices and the continued fraction should be replaced by a continued fraction of 2×2 matrices, i.e. the continued fraction becomes a matrix continued fraction.

In CS basis representation (22) turns into a homogeneous algebraic equation

$$((\underline{g}_{FV0}^C(E))^{-1} - \underline{v}_{FV0}^{(s)})\underline{\psi} = 0, \quad (25)$$

which is solvable if the determinant is zero

$$|(\underline{g}_{FV0}^C(E))^{-1} - \underline{v}_{FV0}^{(s)}| = 0. \quad (26)$$

5. Numerical illustrations

In this work we use units such that $\hbar = 1$, $m = 1$, $e^2 = 1$, and $c = 137.03602$. We consider first the hydrogen atom with $Z = -1$ and $l = 0$. The table below show the exact non-relativistic and relativistic Klein-Gordon hydrogen energies, as well as the numerical results of the FV0 equations. We found that the numerical zeros of the determinant in (26) coincide with the exact Klein-Gordon hydrogen eigenstates up to 10 digits, even for higher excited states, irrespective of N .

Then we add a short-range potential

$$v^{(s)} = v_0 e^{-\alpha_0 r} / r \quad (27)$$

with $v_0 = 2$ and $\alpha_0 = 2$, and investigate its effect on the bound states. The results are shown in the last column. We found that the method is accurate enough to give account of the fine relativistic effects. We also experienced a rapid convergence in N , the number of states used in the expansion. The rate of convergence was similar that we observed in the non-relativistic case in Ref. [40].

6. Summary and conclusions

In this work we considered a relativistic spin-0 particle in a Coulomb plus short-range potential. We adopted the Feshbach-Villars formalism. In this formalism the Klein-Gordon wave function is split into two components and for the component we get a Schrödinger-like equation with a non-hermitian Hamiltonian. We have rewritten the equations into a Lippmann-Schwinger form and represented the short-range part of the potential in CS basis by a finite matrix. We calculated the CS matrix elements Feshbach-Villars Coulomb Green's operator by a matrix continued fraction. This representation of the Green's operator is exact, thus even a small basis representation gives a faithful account of the whole spectra of the Klein-Gordon hydrogen atom. The method gives very accurate results for the Coulomb plus short-range case as well.

n	Sch+ v^C	KG+ v^C	FV0+ v^C	FV0+ v^C+v^s
0	-0.50000000	-0.50003329	-0.50003329	-0.28203629
1	-0.12500000	-0.12500541	- 0.12500541	-0.09299089
2	-0.05555556	-0.05555728	- 0.05555728	-0.04546869
3	-0.03125000	-0.03125075	-0.03125075	-0.02685280
4	-0.02000000	-0.02000039	-0.02000039	-0.01770225
5	-0.01388889	-0.01388912	-0.01388912	-0.01254053
6	-0.01020408	-0.01020423	-0.01020423	-0.00934633
7	-0.00781250	-0.00781260	-0.00781260	-0.00723344
8	-0.00617284	-0.00617291	-0.00617291	-0.00576369
9	-0.00500000	-0.00500005	-0.00500005	-0.00470027
10	-0.00413223	-0.00413227	-0.00413227	-0.00390614

Table 1. Feshbach-Villars eigenstates of hydrogen atom (FV0+ v^C), hydrogen plus short range potential (FV0+ $v^C + v^s$) compared to the exact Klein-Gordon (KG+ v^C) and Schrödinger (Sch+ v^C) results.

This is another example of non-hermitian quantum mechanics [43]. The FV0 Hamiltonian is not hermitian, yet it has real eigenvalues. It is hermitian in a generalized sense [10, 14]. Interestingly, Feshbach-Villars equations can also be derived by requiring CPT symmetry for the quantum mechanical equation [13].

The solution of the Feshbach-Villars equations pose a real challenge to most of the solution methods due to the long-range-type kinetic energy in the coupling term. However, we can wrap up the infinite block-tridiagonal matrix into the Green's matrix by using matrix continued fractions thus eliminating the main hurdle of working with Feshbach-Villars equations.

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